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FILE COVERS 1907 - 15 Feb 2002 VOL 136 ISS 8  
FILE LAST UPDATED: 14 Feb 2002 (20020214/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

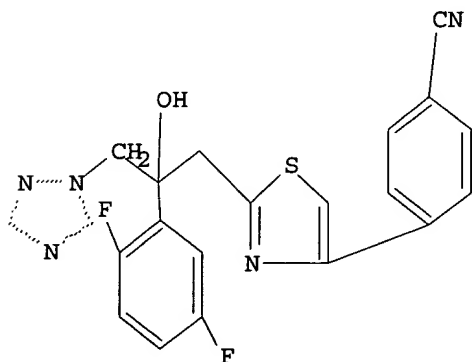
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The P indicator for Preparations was not generated for all of the CAS Registry Numbers that were added to the CAS files between 12/27/01 and 1/23/02. As of 1/23/02, the situation has been resolved. Searches and/or SDIs in the H/Z/CA/CAPLUS files incorporating CAS Registry Numbers with the P indicator executed between 12/27/01 and 1/23/02 may be incomplete. See the NEWS message on this topic for more information.

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Structure attributes must be viewed using STN Express query preparation.

L3 87 SEA FILE=REGISTRY SSS FUL L1

L4 2 SEA FILE=CAPLUS L3

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L4 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:338523 CAPLUS

DOCUMENT NUMBER: 134:353309

TITLE: Synthesis and formulation of N-substituted carbamoyloxyalkyl-azolium derivatives and their use

as

antifungal agents

INVENTOR(S): Fukuda, Hiroshi; Hayase, Tadakatsu; Mizuguchi, Eisaku;

Shimma, Nobuo; Ohwada, Jun; Oikawa, Nobuhiro; Sakaitani, Masahiro; Tsukazaki, Masao; Umeda, Isao F. Hoffmann-La Roche A.-G., Switz.

PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 83 pp.

CODEN: PIXXD2

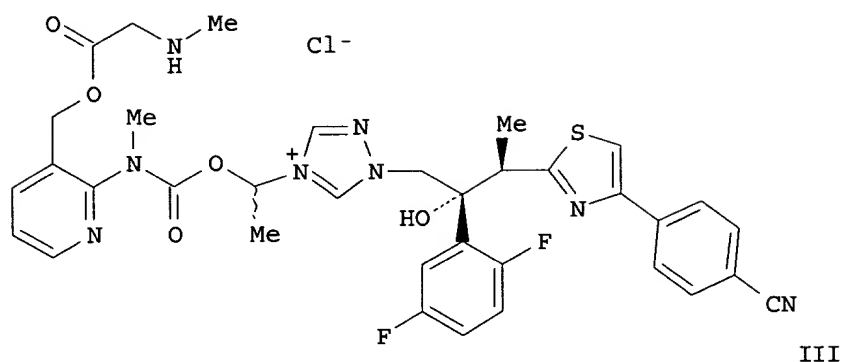
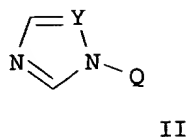
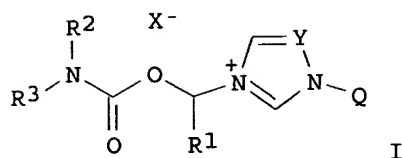
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032652	A2	20010510	WO 2000-EP10524	20001025
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.:			EP 1999-121694	A 19991102
OTHER SOURCE(S):		MARPAT 134:353309		
GI				



AB The synthesis and use of N-substituted carbamoyloxyalkyl-azolium derivs. of general formula I are claimed as antifungal agents [wherein Q is a group of an antifungal azole of formula II; Y is N or CH; R1 is H or alkyl; R2 is H, alkyl, alkylcarbonyloxyalkyl, alkoxy carbonyl, alkylcarbonyl, mono- or dialkylaminoalkylcarbonyloxyalkyl; R3 is alkylaminoalkyl, alkylcarbonyl(oxy)alkyl, optionally substituted Ph, pyridin-2-yl, etc. or the group R2R3N may form an optionally substituted pyrrolidine, pyrrolidone or piperidine; X- is a pharmaceutically acceptable anion]. For instance, the synthesis of III occurs via the alkylation of 1-[(2R,3R)-3-[4-(4-cyanophenyl)thiazol-2-yl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-[1,2,4]-triazole (IV, prepd. in 8 steps) with N-methyl-N-(3-[(N-tert-butoxycarbonyl-N-methylamino)acetoxy)methyl]pyridin-2-yl]carbamic acid 1-chloroethyl ester (prepd. from 2-chloronicotinic acid) in CH3CN with NaI at 45-50.degree.C for 15 h. Deprotection of the resulting salt with HCl led to the isolation of III as the dihydrochloride salt. Soly. of the invention compds. was detd. in distd. water and said to be greater than known antimycotic azoles of formula II. In particular, III soly. in water and physiol. saline was >1000 mg/mL. Representative compds. I were incubated with human plasma (10 .mu.g/mL) at 37.degree.C up to 2 h resulting in degrdn. to common metabolite IV in <6 min (6 exs.). Antifungal activity of compds. I and Fluconazole and Itraconazole was detd. in male Fisher rats infected with *C. albicans* or *A. fumigatus* administered i.v. and p.o. ED50 (.mu.mol/kg) for III was 2.8 (i.v.) and 7 (p.o.) against *C. albicans* UTHS93-2067 vs. 8.1 for Fluconazole and 4.2 for Itraconazole (both p.o.). A description of an i.m., gelatin capsule and tablet formulation are provided as well as detailed HPLC anal. data for representative compds. Azolium salts I are for the prophylaxis and/or treatment of fungal infections.

IT 338990-72-0P 338990-80-0P 338990-81-1P  
 338990-82-2P 338990-84-4P 338990-94-6P  
 338990-99-1P 338991-04-1P 338991-05-2P

338991-10-9P 339307-64-1P

RL: BAC (Biological activity or effector, except adverse); IMF

(Industrial

manufacture); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis of N-substituted carbamoyloxyalkyl-azolium derivs. and their use as antifungal agents)

IT 22916-47-8DP, Miconazole, derivs. of 65277-42-1DP, Ketoconazole, derivs.

of 84625-61-6DP, Itraconazole, derivs. of 136067-84-0DP, derivs. of 136657-97-1DP, derivs. of 149715-95-7DP, derivs. of 151856-47-2DP, derivs. of 155432-64-7DP, derivs. of 182760-06-1DP, derivs. of 213381-02-3DP, derivs. of 241479-66-3DP, derivs. of 241479-67-4DP, derivs. of 241479-68-5DP, derivs. of

338990-73-1P 338990-74-2P 338990-75-3P

338990-76-4P 338990-77-5P 338990-78-6P

338990-79-7P 338990-83-3P 338990-85-5P

338990-86-6P 338990-87-7P 338990-88-8P

338990-89-9P 338990-90-2P 338990-91-3P

338990-92-4P 338990-93-5P 338990-95-7P

338990-96-8P 338990-97-9P 338990-98-0P

338991-00-7P 338991-01-8P 338991-02-9P

338991-03-0P 338991-06-3P 338991-07-4P

338991-08-5P 338991-09-6P 338991-11-0P

338991-12-1P 338991-13-2P 338991-14-3P

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338991-48-3P 338991-49-4P 338991-50-7P

338991-51-8P 338991-52-9P 338991-53-0P

RL: BAC (Biological activity or effector, except adverse); IMF

(Industrial

manufacture); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

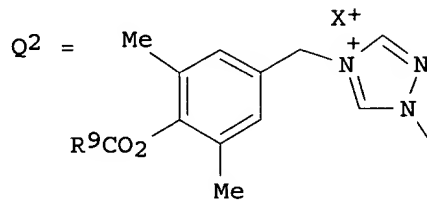
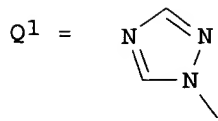
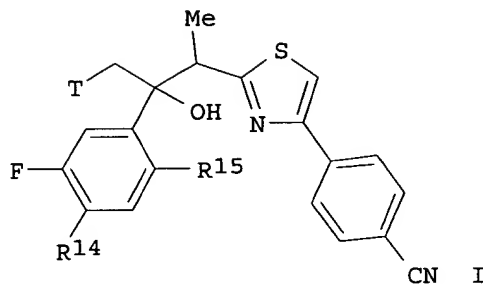
(synthesis of N-substituted carbamoyloxyalkyl-azolium derivs. and their use as antifungal agents)

IT 2258-42-6P, Acetic formic anhydride 14667-47-1P, Methyl 2-aminonicotinate 29055-08-1P 32399-12-5P, 2-(N-Methylamino)-3-hydroxymethylpyridine 49609-84-9P, 2-Chloronicotinoyl chloride 122734-34-3P 186353-05-9P, Chloromethyl N-Methyl-N-(phenyl)carbamate 232951-83-6P, tert-Butyl 2-chloronicotinate 338990-20-8P, Chloromethyl N-Methyl-N-(2-(acetoxymethyl))phenylcarbamate 338990-21-9P, 1-Chloroethyl N-Methyl-N-(3-(acetoxymethyl)pyridin-2-yl)carbamate 338990-22-0P, 1-Chloroethyl N-Acetyl-N-methylcarbamate 338990-23-1P, 2(S)-Acetoxymethyl-1-(chloromethyloxycarbonyl)pyrrolidine 338990-24-2P, Chloromethyl N-Methyl-N-(2-acetoxyethyl)carbamate 338990-25-3P, N-Methyl-N-(3-acetoxypentyl)carbamate 338990-26-4P, N-(2-Methylphenyl)-N-(2-acetoxyethyl)carbamate 338990-27-5P 338990-28-6P 338990-29-7P 338990-30-0P, N-Methyl-N-(2-((N-(tert-butoxycarbonyl)-N-(methylamino)methyl)phenyl)carbamate 338990-31-1P, N-Methyl-N-(3-((N-(tert-butoxycarbonyl)-N-methylamino)acetoxymethyl)pyridin-2-yl)carbamate 338990-32-2P 338990-33-3P 338990-34-4P 338990-35-5P 338990-36-6P 338990-37-7P 338990-38-8P 338990-39-9P 338990-40-0P 338990-41-1P 338990-42-2P 338990-43-3P 338990-44-4P 338990-45-5P 338990-46-6P 338990-47-7P 338990-48-8P 338990-49-9P 338990-50-0P 338990-51-1P 338990-52-2P 338990-53-3P 338990-54-4P 338990-55-5P 338990-56-6P 338990-57-7P 338990-58-8P 338990-59-9P 338990-60-0P 338990-61-1P 338990-62-2P 338990-63-3P 338990-64-4P 338990-65-5P 338990-66-6P 338990-67-7P 338990-68-8P 338990-69-9P 338990-70-0P 338990-71-1P 338990-72-2P 338990-73-3P 338990-74-4P 338990-75-5P 338990-76-6P 338990-77-7P 338990-78-8P 338990-79-9P 338990-80-0P 338990-81-1P 338990-82-2P 338990-83-3P 338990-84-4P 338990-85-5P 338990-86-6P 338990-87-7P 338990-88-8P 338990-89-9P 338990-90-0P 338990-91-1P 338990-92-2P 338990-93-3P 338990-94-4P 338990-95-5P 338990-96-6P 338990-97-7P 338990-98-8P 338990-99-9P 338990-100-0P 338990-101-1P 338990-102-2P 338990-103-3P 338990-104-4P 338990-105-5P 338990-106-6P 338990-107-7P 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**338990-62-8P 338990-63-9P 338990-64-0P**  
**338990-65-1P** 338990-66-2P, Isopropyl-(2-nitrobenzyl)carbamic  
 acid tert-butyl ester 338990-67-3P, Isopropyl(2-Aminobenzyl)carbamic  
 acid tert-butyl ester 338990-68-4P, Isopropyl-(2-  
 methylaminobenzyl)carbamic acid tert-butyl ester 338990-70-8P,  
 tert-Butyl 2-(N-methylamino)nicotinate 338990-71-9P, Methyl  
 2-(N-formylamino)nicotinate 338991-54-1P,  
 N-Isopropyl-2-nitrobenzylamine  
 338991-55-2P  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic  
 preparation); PREP (Preparation)  
 (synthesis of N-substituted carbamoyloxyalkyl-azolium derivs. and  
 their use as antifungal agents)  
 IT **241479-67-4P**, 1-[(2R,3R)-3-[4-(4-Cyanophenyl)thiazol-2-yl]-2-(2,5-  
 difluorophenyl)-2-hydroxybutyl]-[1,2,4]-triazole  
 RL: MFM (Metabolic formation); RCT (Reactant); SPN (Synthetic  
 preparation); BIOL (Biological study); FORM (Formation, nonpreparative);  
 PREP (Preparation)  
 (synthesis of N-substituted carbamoyloxyalkyl-azolium derivs. and  
 their use as antifungal agents)  
 L4 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1999:576927 CAPLUS  
 DOCUMENT NUMBER: 131:199700  
 TITLE: Preparation of 3-[4-(4-cyanophenyl)thiazol-2-yl]-1-  
 (1H-1,2,4-triazol-1-yl)-butan-2-ols as antifungals.  
 INVENTOR(S): Hayase, Tadakatsu; Ichihara, Shigeyasu; Isshiki,  
 Yoshiaki; Liu, Pingli; Ohwada, Jun; Sakai, Toshiya;  
 Shimma, Nobuo; Tsukazaki, Masao; Umeda, Isao;  
 Yamazaki, Toshikazu  
 PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.  
 SOURCE: PCT Int. Appl., 68 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9945008	A1	19990910	WO 1999-EP1327	19990301
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ,			
TM				
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG		
AU 9929313	A1	19990920	AU 1999-29313	19990301

US 6300353 B1 20011009 US 1999-263027 19990305  
 PRIORITY APPLN. INFO.: EP 1998-104036 A 19980306  
 EP 1998-123310 A 19981208  
 EP 1999-101360 A 19990126  
 WO 1999-EP1327 W 19990301  
 OTHER SOURCE(S): MARPAT 131:199700  
 GI



AB Title compds. [I; R<sub>14</sub>, R<sub>15</sub> = H, F; T = Q<sup>1</sup>, Q<sup>2</sup>; R<sub>9</sub> = pyrrolidinyl, ANHB; A = H, alkyl; B = alkylene, CH<sub>2</sub>CONHCH<sub>2</sub>, (CH<sub>2</sub>)<sub>3</sub>CH(NH<sub>2</sub>); X = pharmaceutically acceptable anion], were prepd. Thus,

4-[2-[(1R,2R)-2-(2,5-difluorophenyl)-2-hydroxy-1-methyl-3-(1,2,4-triazol-1-yl)propyl]thiazol-4-yl]benzonitrile (prepn. given) and 4-tert-butoxycarbonylmethylaminoacetoxymethyl-3,5-dimethylbenzyl bromide were refluxed 15 h in MeCN; the product was stirred

with aq. HCl in EtOAc to give 1-[(2R,3R)-3-[4-(4-cyanophenyl)thiazol-2-yl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-4-(3,5-dimethyl-4-methylaminoacetoxymethyl)-1H-1,2,4-triazol-4-ium bromide (II). II inhibited candidiasis in rats with ED<sub>50</sub> = 5.3 .mu.mol/kg. Drug formulations contg. II are given.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

#### FORMAT

IT 241479-18-5P 241479-20-9P 241479-21-0P  
 241479-23-2P 241479-24-3P 241479-26-5P 241479-27-6P  
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 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
 (prepn. of cyanophenylthiazolyltriazolylbutanols as antifungals)  
 IT 20099-89-2P, 2-Bromo-4'-cyanoacetophenone 135206-87-0P 135270-08-5P  
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 241479-87-8P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of cyanophenylthiazolyltriazolylbutanols as antifungals)

=> file uspatfull

FILE 'USPATFULL' ENTERED AT 14:04:26 ON 15 FEB 2002  
 CA INDEXING COPYRIGHT (C) 2002 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 14 Feb 2002 (20020214/PD)  
 FILE LAST UPDATED: 14 Feb 2002 (20020214/ED)  
 HIGHEST GRANTED PATENT NUMBER: US6330719  
 HIGHEST APPLICATION PUBLICATION NUMBER: US2002019999  
 CA INDEXING IS CURRENT THROUGH 14 Feb 2002 (20020214/UPCA)  
 ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 14 Feb 2002 (20020214/PD)  
 REVISED CLASS FIELDS (/NCL) LAST RELOADED: Dec 2001  
 USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Dec 2001

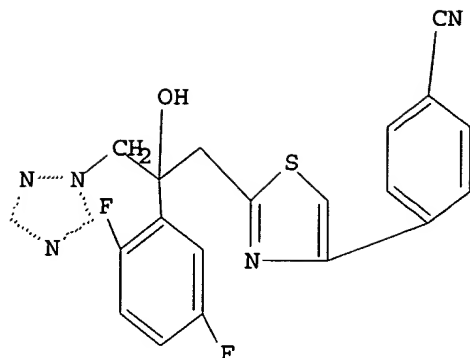
>>> Page images are available for patents from 1/1/1998. Patents <<<  
 >>> and applications are typically loaded on the day of publication.<<<  
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 >>> Image data for the /FA field are available the following update.<<<

>>> Complete CA file indexing for chemical patents (or equivalents) <<<  
 >>> is included in file records. A thesaurus is available for the <<<  
 >>> USPTO Manual of Classifications in the /NCL, /INCL, and /RPCL <<<  
 >>> fields. This thesaurus includes catchword terms from the <<<  
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 >>> the /IC5 and /IC fields include the corresponding catchword <<<  
 >>> terms from the IPC subject headings and subheadings. <<<

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d que

L1 STR



Structure attributes must be viewed using STN Express query preparation.

L3 87 SEA FILE=REGISTRY SSS FUL L1

L5 1 SEA FILE=USPATFULL L3

=> d 15 ibib abs hitstr

L5 ANSWER 1 OF 1 USPATFULL

ACCESSION NUMBER: 2001:173607 USPATFULL

TITLE: Azoles for treatment of fungal infections

INVENTOR(S): Hayase, Tadakatsu, Chigasaki, Japan  
 Ichihara, Shigeyasu, Kawasaki, Japan  
 Isshiki, Yoshiaki, Chigasaki, Japan  
 Liu, Pingli, Fujisawa, Japan  
 Ohwada, Jun, Kamakura, Japan  
 Sakai, Toshiya, Fujisawa, Japan  
 Shimma, Nobuo, Chigasaki, Japan  
 Tsukazaki, Masao, Fujisawa, Japan  
 Umeda, Isao, Yokohama, Japan  
 Yamazaki, Toshikazu, Kamakura, Japan  
 PATENT ASSIGNEE(S): Basilea Pharmaceutica AG, a Swiss Company, Basel, Switzerland (non-U.S. corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 6300353	B1	20011009
APPLICATION INFO.:	US 1999-263027		19990305 (9)

	NUMBER	DATE
PRIORITY INFORMATION:	EP 1998-104036	19980306
	EP 1998-123310	19981208
	EP 1999-101360	19990126

DOCUMENT TYPE: Utility

FILE SEGMENT: GRANTED

PRIMARY EXAMINER: Gerstl, Robert

LEGAL REPRESENTATIVE: Johnston, George W., Tramaloni, Dennis P.

NUMBER OF CLAIMS: 37

EXEMPLARY CLAIM: 1

LINE COUNT: 1686

CAS INDEXING IS AVAILABLE FOR THIS PATENT.



AB Azole derivatives of the formula I ##STR1##

wherein

R.sup.14, R.sup.15 are each independently hydrogen or fluorine,

T is a group of the formula: ##STR2##

wherein

R.sup.9 is pyrrolidinyl or a group A--NH--B--,

A is hydrogen or straight-chain or branched C.sub.1 -C.sub.5 alkyl;

B is straight-chain or branched C.sub.1 -C.sub.4 alkylene, --CH.sub.2 --CONH--CH.sub.2 or --CH.sub.2 CH.sub.2 CH.sub.2 --CH(NH.sub.2); and

X.sup.- is a pharmaceutically acceptable anion;

and pharmaceutically acceptable salts of said compounds, and hydrates and solvates of the compounds of formula I and the salts thereof can be used in the production of medicaments for treating fungal infections

and

mycoses.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

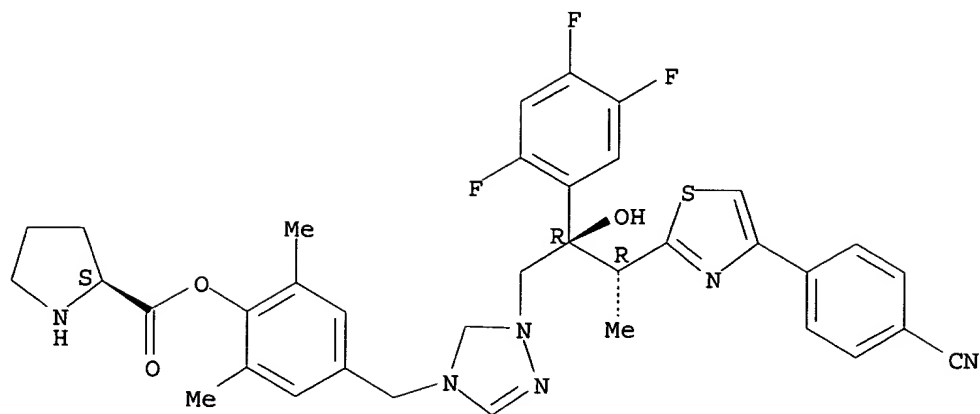
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241479-66-3P 241479-67-4P

(prepn. of cyanophenylthiazolyltriazolylbutanols as antifungals)

RN 241479-18-5 USPATFULL

CN L-Proline, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-20-9 USPATFULL

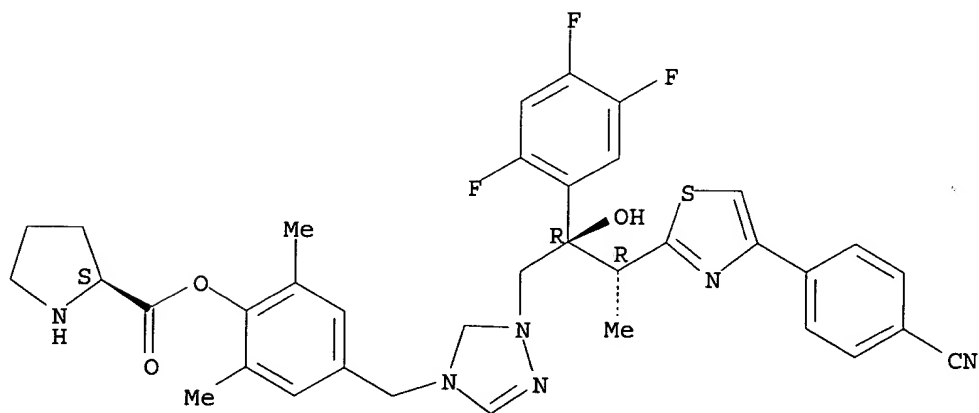
CN L-Proline, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-19-6

CMF C36 H34 F3 N6 O3 S

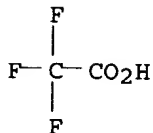
Absolute stereochemistry.

**FRAGMENT DIAGRAM IS INCOMPLETE**

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CRN 76-05-1

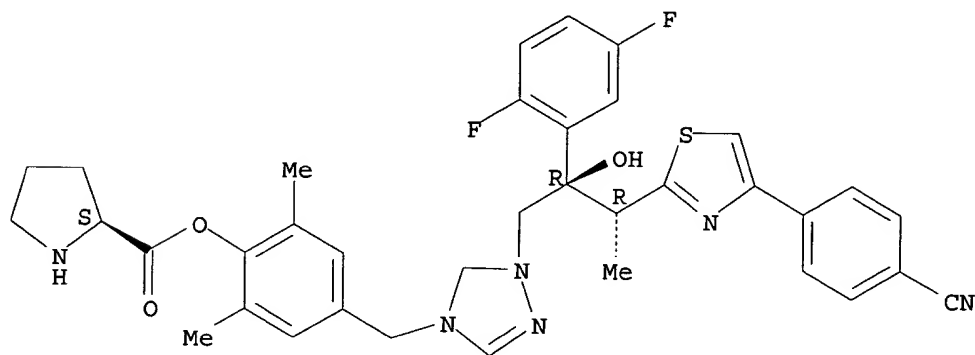
CMF C2 H F3 O2



RN 241479-21-0 USPATFULL

CN L-Proline, 4-[[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● Br<sup>-</sup>

FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-23-2 USPATFULL

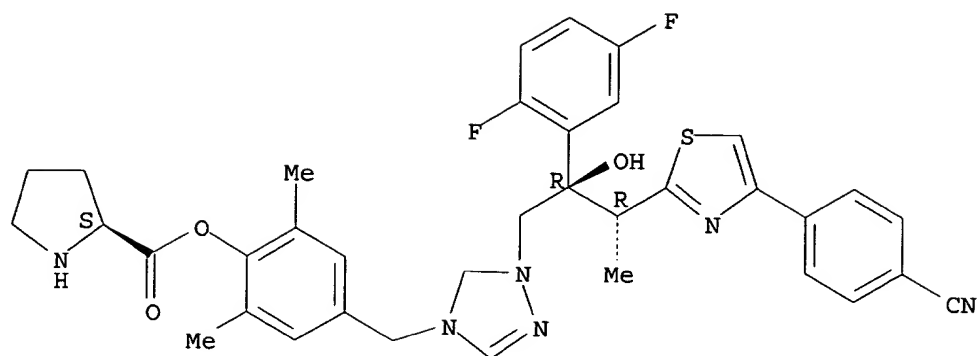
CN L-Proline, 4-[[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-22-1

CMF C36 H35 F2 N6 O3 S

Absolute stereochemistry.

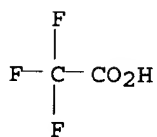


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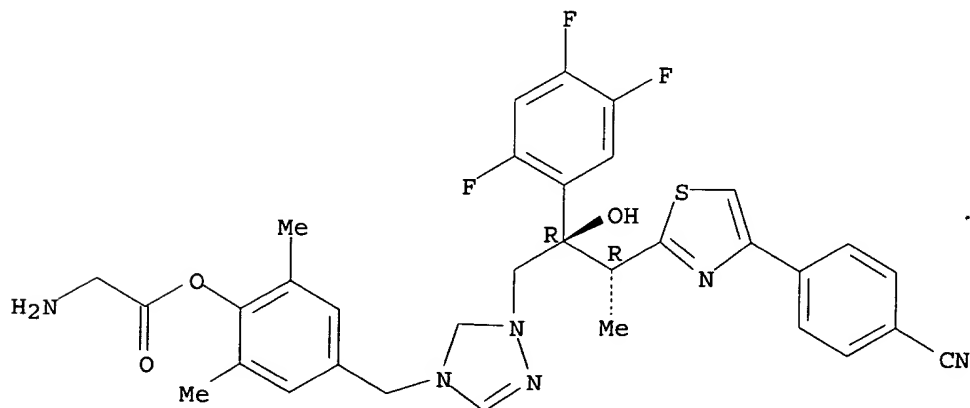
CMF C2 H F3 O2



RN 241479-27-6 USPATFULL

CN Glycine, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br<sup>-</sup>

**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-29-8 USPATFULL

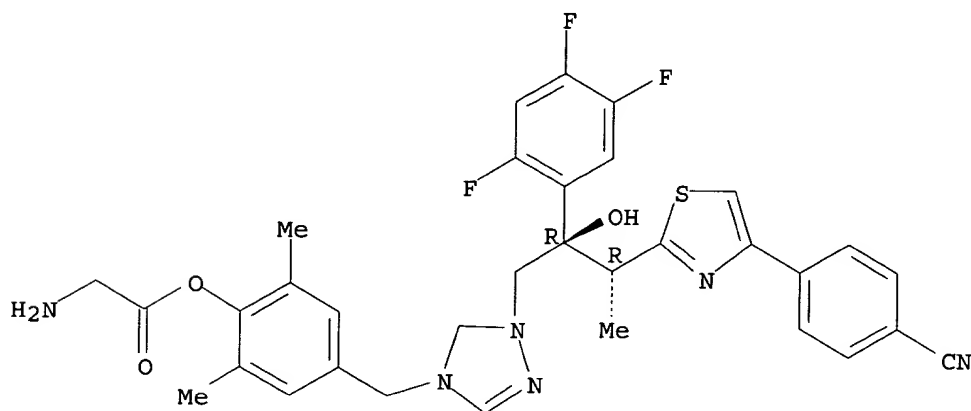
CN Glycine, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-28-7

CMF C33 H30 F3 N6 O3 S

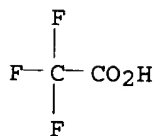
Absolute stereochemistry.

**FRAGMENT DIAGRAM IS INCOMPLETE**

CM 2

CRN 76-05-1

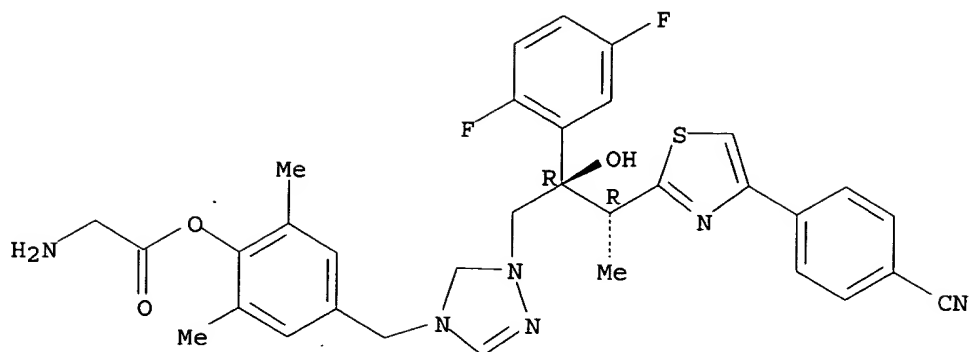
CMF C2 H F3 O2



RN 241479-30-1 USPATFULL

CN Glycine, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br<sup>-</sup>

**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-32-3 USPATFULL

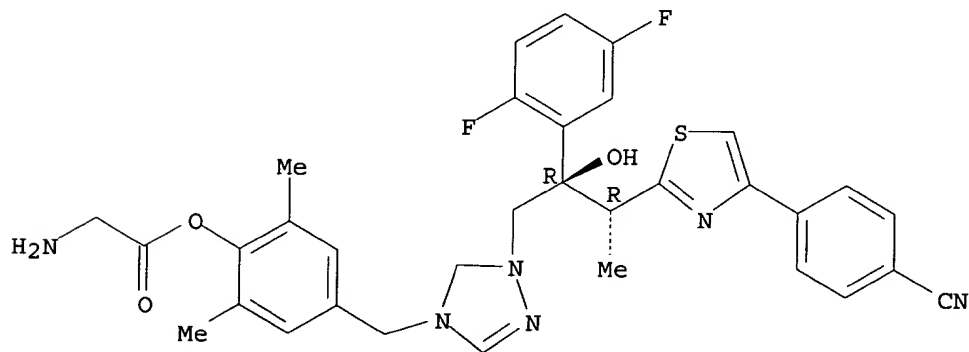
CN Glycine, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-31-2

CMF C33 H31 F2 N6 O3 S

Absolute stereochemistry.

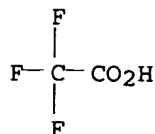


**FRAGMENT DIAGRAM IS INCOMPLETE**

CM 2

CRN 76-05-1

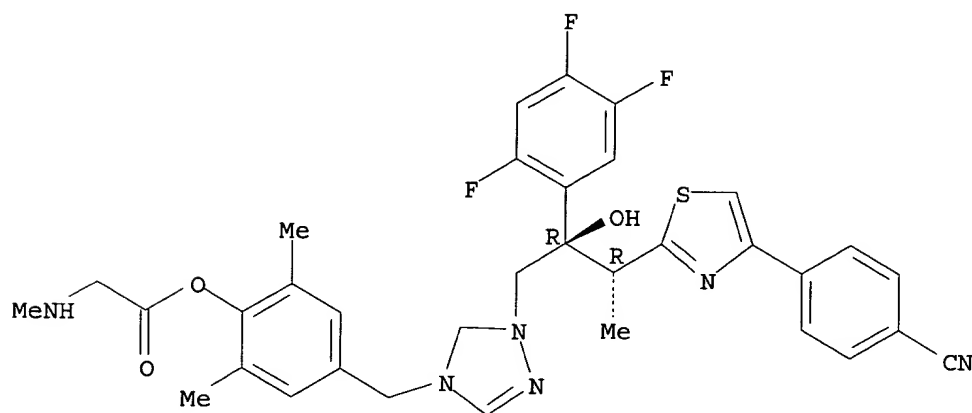
CMF C2 H F3 O2



RN 241479-36-7 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-38-9 USPATFULL

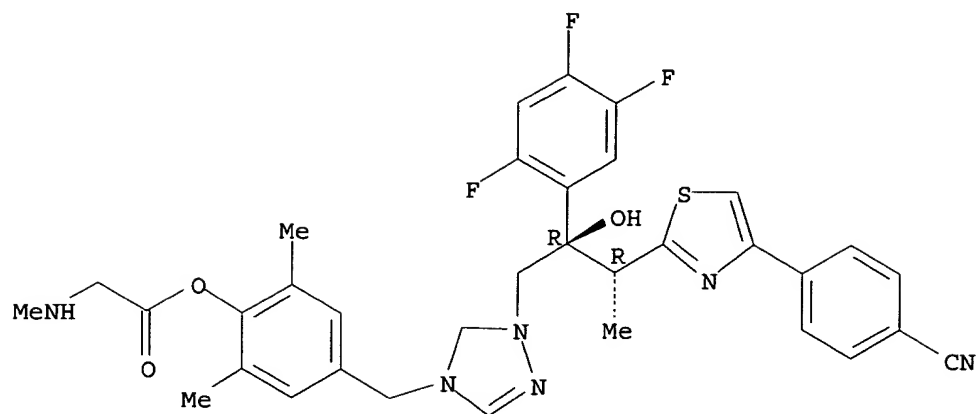
CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-37-8

CMF C34 H32 F3 N6 O3 S

Absolute stereochemistry.

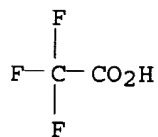


FRAGMENT DIAGRAM IS INCOMPLETE

CM 2

CRN 76-05-1

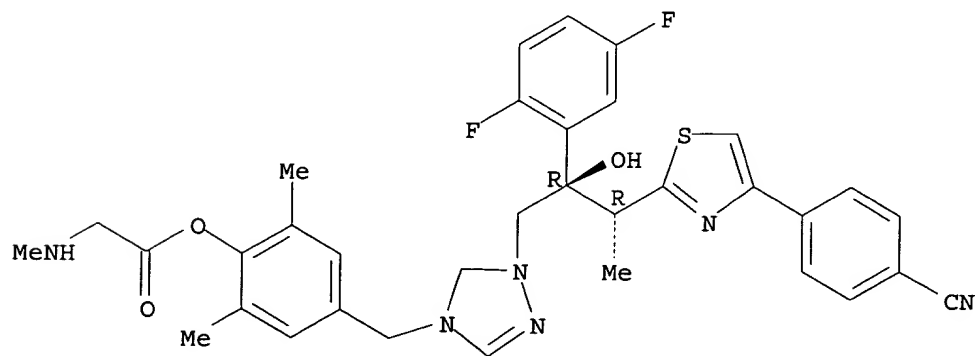
CMF C2 H F3 O2



RN 241479-39-0 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br<sup>-</sup>



**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-41-4 USPATFULL

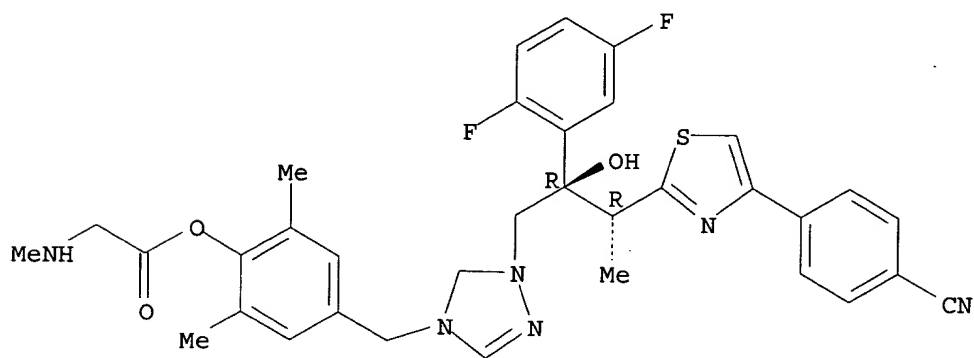
CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI)  
(CA INDEX NAME)

CM 1

CRN 241479-40-3

CMF C34 H33 F2 N6 O3 S

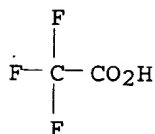
Absolute stereochemistry.

**FRAGMENT DIAGRAM IS INCOMPLETE**

CM 2

CRN 76-05-1

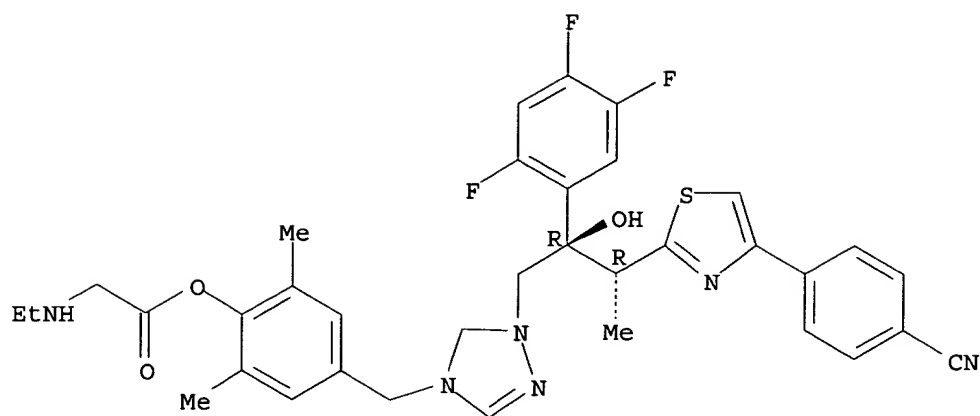
CMF C2 H F3 O2



RN 241479-45-8 USPATFULL

CN Glycine, N-ethyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br<sup>-</sup>

**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-47-0 USPATFULL

CN Glycine, N-ethyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-

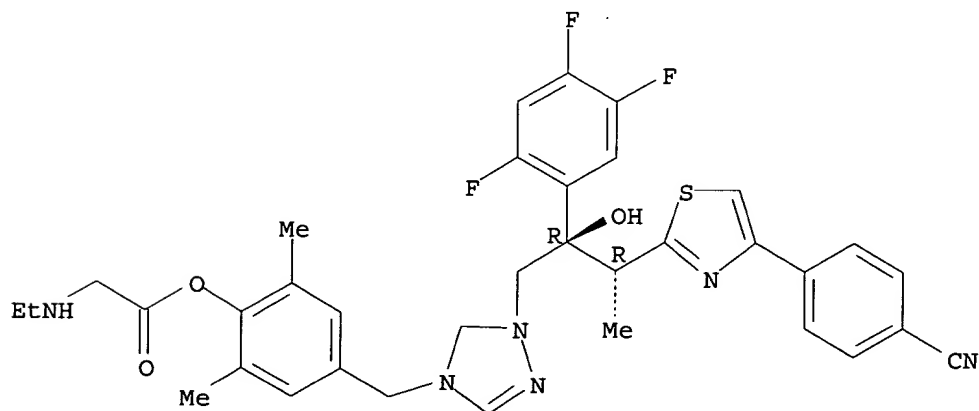
hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-  
2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI)  
(CA INDEX NAME)

CM 1

CRN 241479-46-9

CMF C35 H34 F3 N6 O3 S

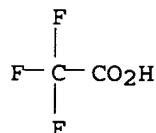
Absolute stereochemistry.



**FRAGMENT DIAGRAM IS INCOMPLETE**

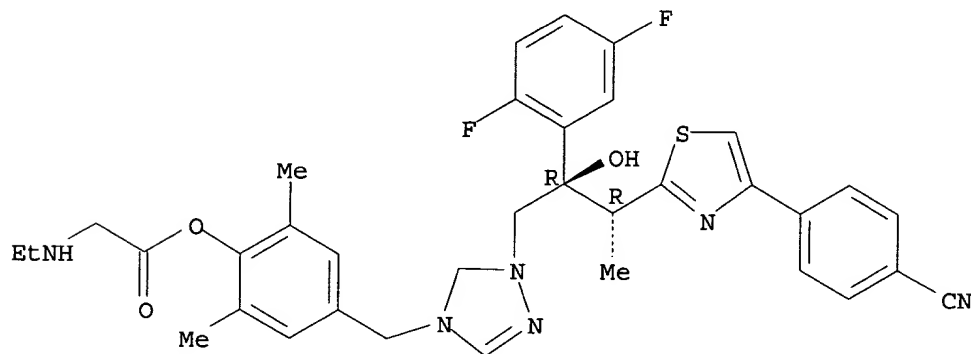
CM 2

CRN 76-05-1  
CMF C2 H F3 O2



RN 241479-48-1 USPATFULL  
CN Glycine, N-ethyl-,  
4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Br<sup>-</sup>

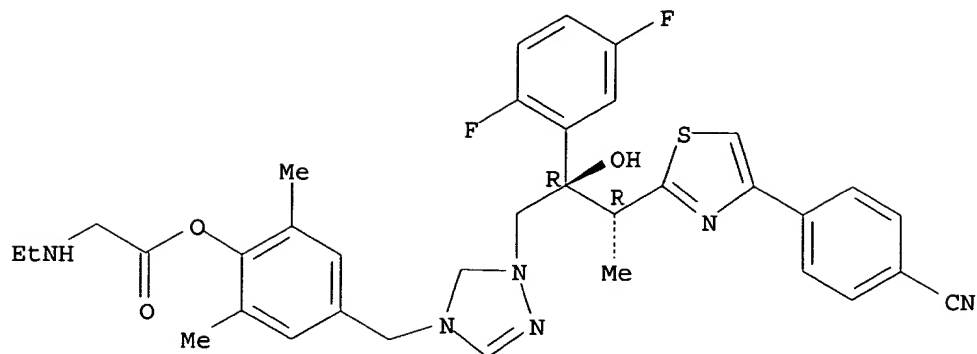
**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-50-5 USPATFULL  
CN Glycine, N-ethyl-,  
4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, mono(trifluoroacetate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 241479-49-2  
CMF C35 H35 F2 N6 O3 S

Absolute stereochemistry.

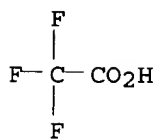


FRAGMENT DIAGRAM IS INCOMPLETE

CM 2

CRN 76-05-1

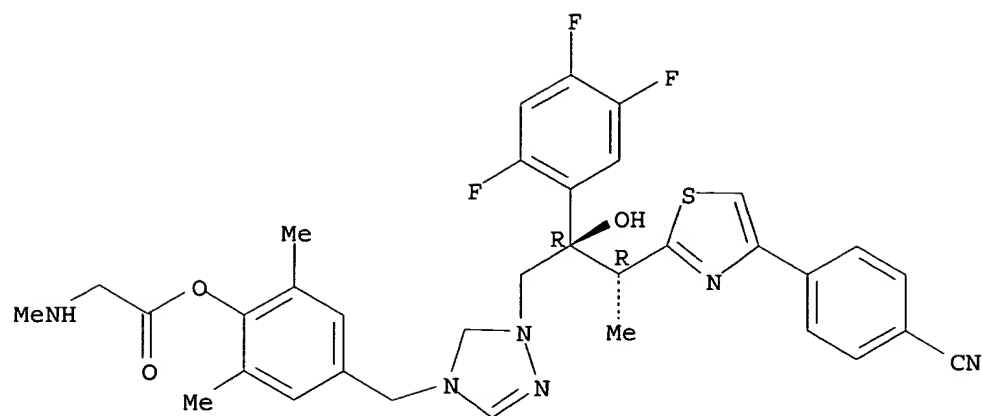
CMF C2 H F3 O2



RN 241479-54-9 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● Cl<sup>-</sup>

**FRAGMENT DIAGRAM IS INCOMPLETE**

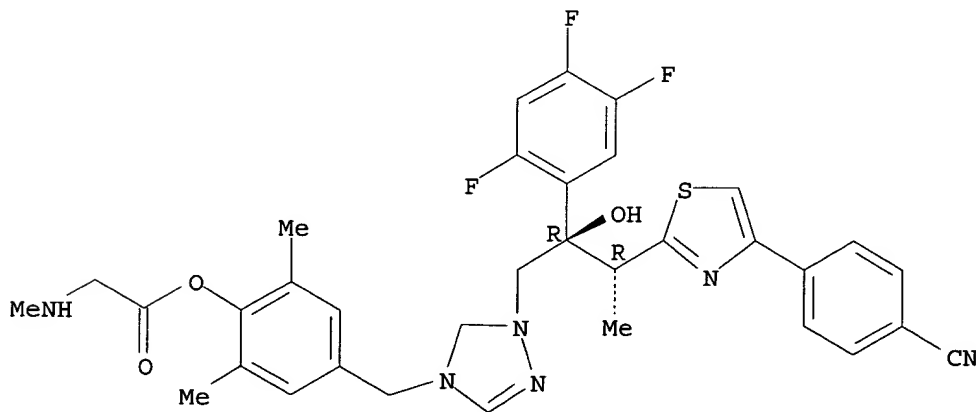
RN 241479-55-0 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-

hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, chloride, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



● Cl<sup>-</sup>

PAGE 2-A

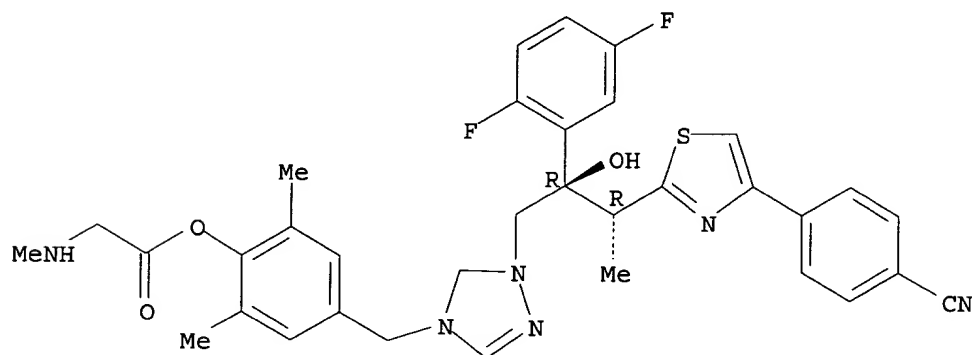
● HCl

**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-56-1 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

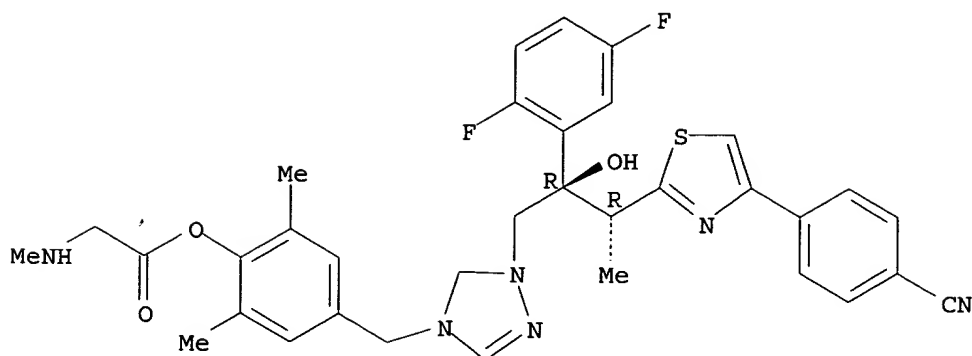
● Cl<sup>-</sup>**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-57-2 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, chloride, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

● Cl<sup>-</sup>

PAGE 2-A

● HCl

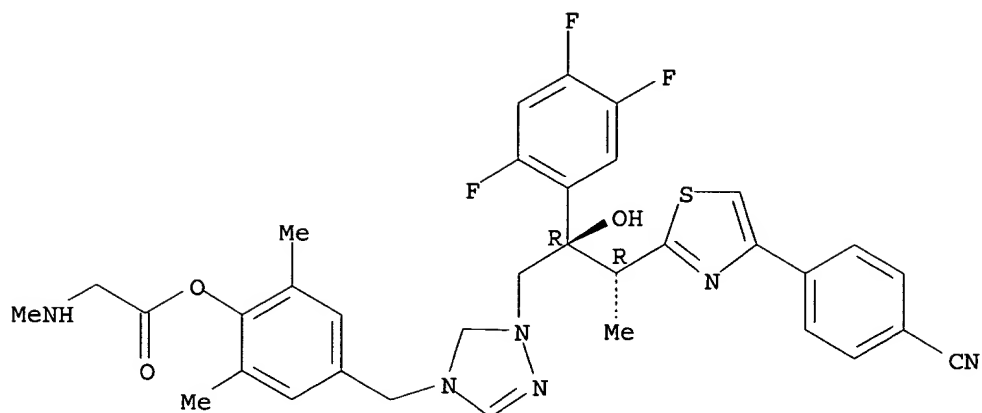
**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-60-7 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

● Br<sup>-</sup>

PAGE 2-A

● HBr

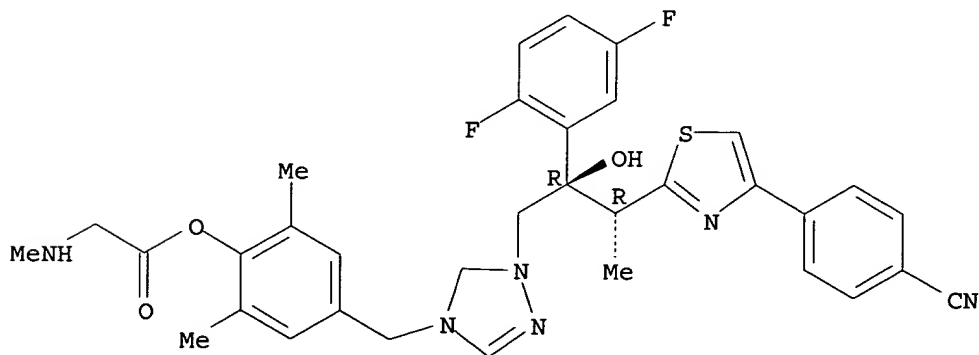
**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-61-8 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, monohydrobromide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

● Br<sup>-</sup>



PAGE 2-A

● HBr

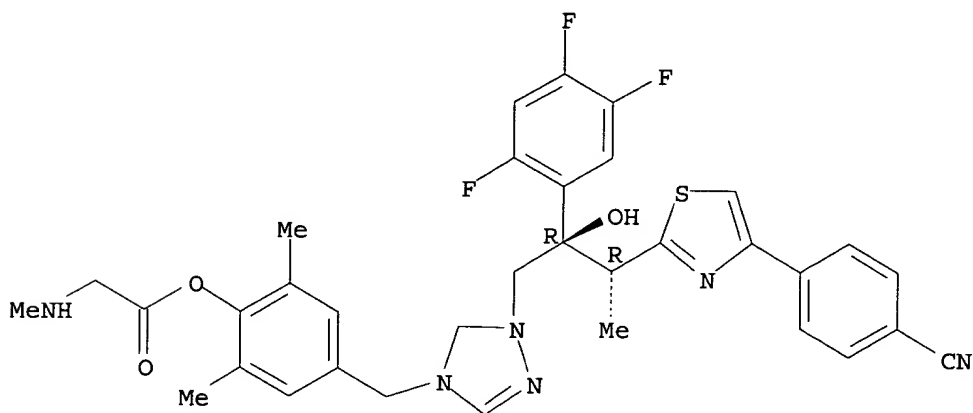
**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-63-0 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

● Br<sup>-</sup>

PAGE 2-A

● HCl

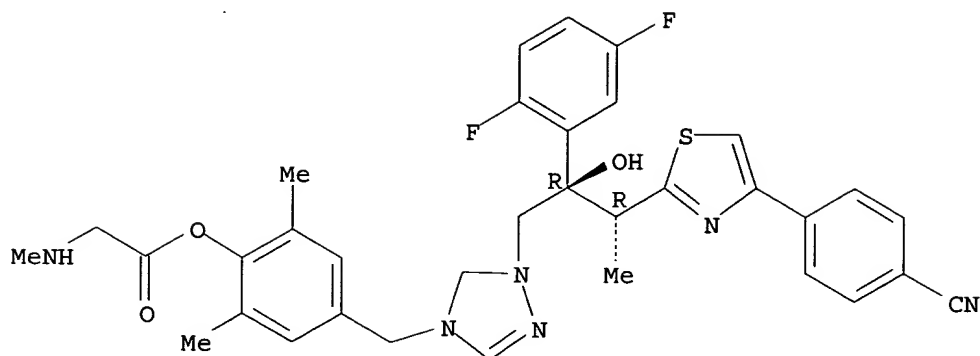
**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-64-1 USPATFULL

CN Glycine, N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,5-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

● Br<sup>-</sup>

PAGE 2-A

● HCl

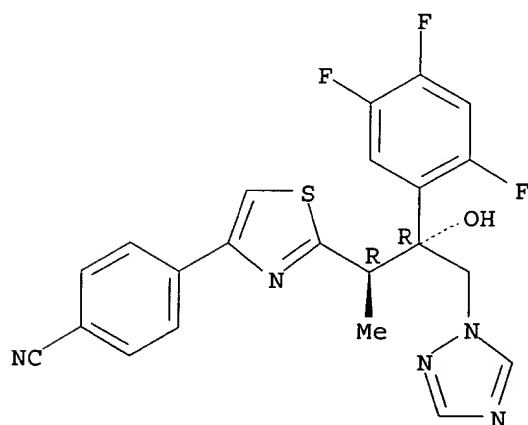
FRAGMENT DIAGRAM IS INCOMPLETE

RN 241479-66-3 USPATFULL

CN Benzonitrile,

4-[2-[(1R,2R)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)-2-(2,4,5-trifluorophenyl)propyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

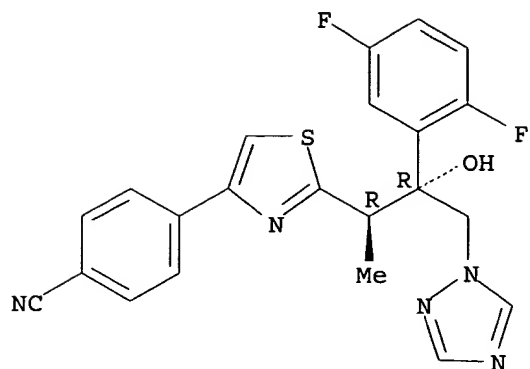
Absolute stereochemistry.



RN 241479-67-4 USPATFULL

CN Benzonitrile, 4-[2-[(1R,2R)-2-(2,5-difluorophenyl)-2-hydroxy-1-methyl-3-(1H-1,2,4-triazol-1-yl)propyl]-4-thiazolyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 241479-83-4P 241479-87-8P

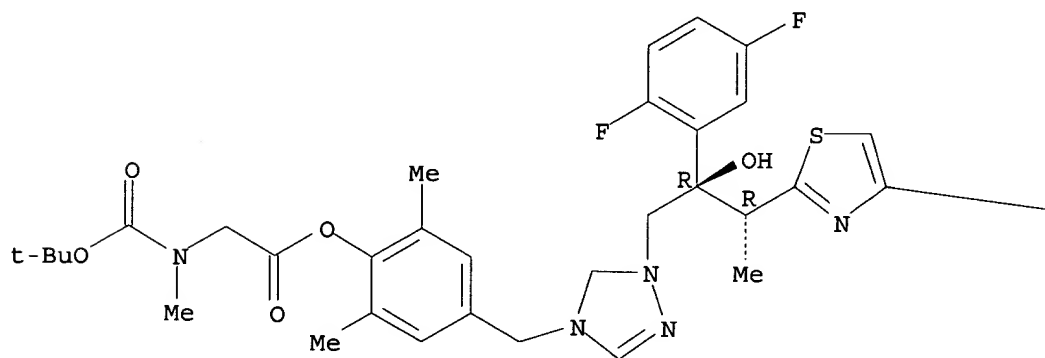
(prepn. of cyanophenylthiazolyltriazolylbutanols as antifungals)

RN 241479-83-4 USPTAFULL

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-N-methyl-, 4-[[1-[[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-(2,6-difluorophenyl)-2-hydroxybutyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide (9CI)  
(CA INDEX NAME)

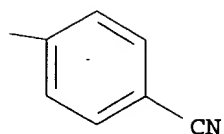
Absolute stereochemistry.

PAGE 1-A



● Br<sup>-</sup>

PAGE 1-B

**FRAGMENT DIAGRAM IS INCOMPLETE**

RN 241479-87-8 USPTFULL

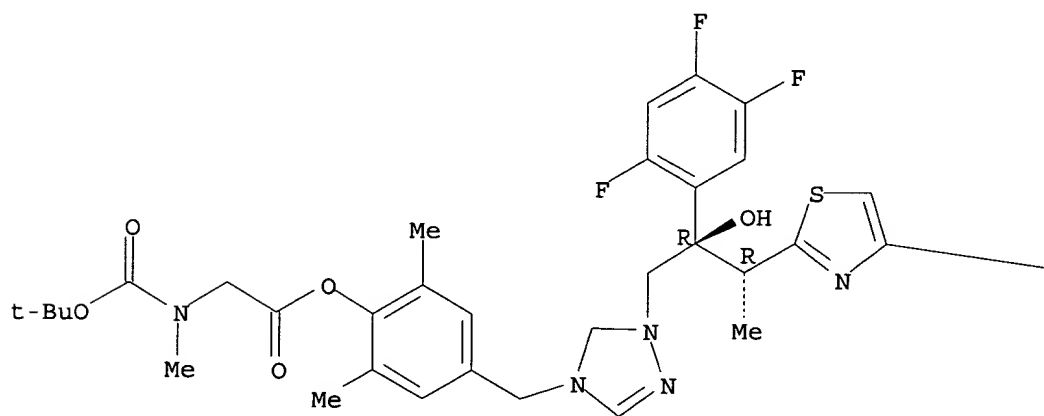
CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-N-methyl-, 4-[[1-[(2R,3R)-3-[4-(4-cyanophenyl)-2-thiazolyl]-2-hydroxy-2-(2,4,5-trifluorophenyl)butyl]-1H-1,2,4-triazolium-4-yl]methyl]-2,6-dimethylphenyl ester, bromide

(9CI)

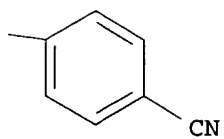
(CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

● Br<sup>-</sup>

PAGE 1-B



FRAGMENT DIAGRAM IS INCOMPLETE